

February 25, 1965

Professor Elbert G. Smith
Department of Chemistry
Mills College
Oakland 13, California

Dear Professor Smith:

Thank you for your interesting letter of February 23.

As I believe I mentioned, I am not so much interested in the merits of DENDRAL as a general notation system as I am in (1) its utility as part of a hypothesis generator, and (2) in the exposure of some of the basic mathematical principles that underlie chemical graphs. In order to accomplish these functions the system was designed to manipulate the most primitive symbols, namely, the individual atoms and types of link between them, and I purposely stayed away from the chemically more interesting conjunctions that constitute the effective functional groups. However, insofar as the list of interesting functions is likely to differ from one application to another, I wonder if the indexing function that you mention in the second paragraph of your letter would not better be accomplished by establishing a property list relevant to the immediate application from the fundamental code. I have not attempted a detailed implementation, but visualize that it would not be too difficult to program the analysis of a list of structures in such a way as to indicate which of them had the requisite functional groups to make them of interest to a particular user. In any case, I would stress that the DENDRAL system is very much computer oriented, and for most of its applications would imply the availability of a fairly substantial computational facility.

The approach to cyclic graphs that I have undertaken is summarized, I now see somewhat clumsily, in an article that appeared in the January 1965 Proceedings of the National Academy of Sciences. I will send you a copy as soon as reprints are available. Briefly, it consists of a general anticipation of the types of trivalent and quadrivalent cyclic graphs on which the actual chemical realizations can be systematically mapped. I am just finishing up on the Part II of the DENDRAL report and will send you a copy at the earliest possibility. If there are some specific questions on the enumeration of these graphs that might be helpful to you at an earlier time, why not let me know by letter or phone and I can send you Xerox copies of some of the tables right away. The enclosed table will give you some idea of the scope of the work now available.

Sincerely yours,

Joshua Lederberg
Professor of Genetics